Available online at www.derpharmachemica.com

ISSN 0975-413X
CODEN (USA): PCHHAX

Der Pharma Chemica, 2016, 8(4):418-424
(http://derpharmachemica.com/archive.html)

CFD Photochemical Modelling in an Urban Street Canyon

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ABSTRACT

The nitrogen oxide gases are subject to fast chemical reactions. The time scales characterizing these reactions are of the order of tens of seconds and thus, comparable with residence time of pollutants in street canyons. The objective of the present study is the performance of small-scale computations for an urban 3D by using a CFD (computational fluid dynamics) code (ANSYS-CFX) to provide steady state wind and pollutant concentration fields. A fast chemistry module simulating chemical reactions taking place within street canyons right after traffic pollutants are emitted is implemented to the model in order to assess the concentrations of NO_x and ozone in space. Circulations created by the city itself and that affect pollutant dispersion are accounted for and hotspot concentrations that depend on street canyon scale effects are also computed. Reactive pollutant dispersion in the street canyon has been numerically investigated using CFD numerical simulation by means of k-ε turbulence model and transport equations for NO, NO_2, and O_3 with simple photochemistry. The area emission source is divided to sub-domains describing NO_x vehicles' emissions. The Background of O_3 was specified, and the gases were allowed to mix and react.

Keywords: Street canyon; Photochemistry; Computational fluid dynamics (CFD); O_3; NOx.

INTRODUCTION

The study on flow and dispersion in urban street canyons have been widely investigate and attracted great concern during the past two decades mainly due to increasing urban pollutants and their adverse impacts on human health. Field measurements and computational fluid dynamics (CFD) techniques are the common tools used to study the flow and pollutants dispersion in street canyons.

The CFD modeling approach as a way to understand street canyon flow and dispersion has become powerful and comprehensive with recent advances in computing power, numerical method/algorithm, and turbulence parameterization. Previous CFD modeling studies have contributed to our understanding of the many important aspects of street canyon flow and dispersion. These include flow regime, dispersion mechanism [2], thermal effects on flow and dispersion [4].

In urban areas, a main pollutant source is automobiles and the pollutants emitted from automobiles, for example NO and NO_2, are chemically reactive. Complex photochemical processes in densely built-up urban areas with traffic often result in a serious air pollution problem. Therefore, to further enhance our understanding of street canyon dispersion, reactive pollutants need to be taken into account.

MATERIALS AND METHODS

2.1. Selected case and simulation

Due to rapid growth of traffic volumes within urban areas, pollutant concentrations are still receiving a lot of attention in densely built-up areas where people are concentrated and where both buildings and the people are more affected.

The street simulated in CFX, is One-way Street, the Width of the street varies with an average value of 10m and with a length of 95m. This street has about 19 building with heights varying between 3m and 18m.

2.1.1. Emission of cars

Traffic emissions in the street are calculated knowing the traffic flow (vehicle/hour) and emission factors (g/km).

The basic formula for estimating emissions, using experimentally (The Core Inventory of Air Emissions in Europe CORINAIR, 3rd Edition 2003 [6]) obtained emission factor is:

Emissions per Period of Time [g] = Emission Factor [g/km] ×Number of Vehicles [veh.] ×Mileage per Vehicle per Period of Time [km/veh.]

The emissions factor depends the vehicle speed (for NOx), with engine capacity CC<1.4 l given as:

$E = 0.5595–0.01047V+10.8e^{-5} V^2$ [g/km].

Where V is the vehicle speed.

2.1.2. Chemical coupling of O_3, NO, and NO_2

The reactive pollutants we are concerned with in this study are nitrogen oxide NO and nitrogen dioxide NO_2, which are supposed to be emitted from automobiles within the street canyon in the presence of background ozone O_3.

The chemical reactions considered are:

NO_2 + sunlight (λ<420nm) → NO + (O^{3p}) (R_0)

(O^{3p}) + O_2 + M → O_3 + M (R_1)

O_3+ NO → NO_2+ O_2 (R_2)

M represents a molecule (N_2 or O_2 or another third molecule).

2.1.3. Reaction rate type

Chemical kinetics characterizes the rate at which chemical species appear or disappear. The kinetic rate constant (of reaction) is a function of temperature and is given in the form:

$$k(T) = AT^{\beta} \exp\left(\frac{-E_a}{RT}\right) \quad (1)$$

This equation is called the Arrhenius equation (used by ANSYS CFX), where A is a pre-exponential factor, β is the temperature exponent, R is the universal gas constant, T is the temperature, and E_a is the activation energy.

2.1.4. Model description

Computational fluid dynamics (CFD) modelling is based on the governing fluid flow and dispersion equations, which are derived from basic conservation and transport principle:

- The mass conservation (continuity) equation.
- The three momentum (Navier-Stokes) equations in x, y, z.
- The transport equation for pollution concentration.

The air within the street canyon can be regarded as an incompressible turbulent flow, and the air and pollutants densities are assumed to be constant. These assumptions are reasonable for lower atmosphere environment as described by Sini et al., 1996 [4].

For the street canyon problem, the standard ***k-ε*** turbulence model governing equations expressed as:

The continuity equation:

$$\frac{\partial U_i}{\partial x_i} = 0 \tag{2}$$

The momentum equation:

$$\frac{\partial U_i}{\partial t} + U_j \frac{\partial U_i}{\partial x_i} = -\frac{1}{\rho}\frac{\partial \bar{p}}{\partial x_i} + \frac{\partial}{\partial x_j}\left(\upsilon \frac{\partial U_i}{\partial x_j} - \overline{u_i' u_j'}\right) \tag{3}$$

k and ε transport equations in the standard ***k-ε*** model:

$$\frac{\partial k}{\partial t} + \vec{V} grad k = div\left(\frac{\upsilon_t}{\sigma_k} grad k\right) + P - \varepsilon \tag{4}$$

$$\frac{\partial \varepsilon}{\partial t} + \vec{V} grad \varepsilon = div\left(\frac{\upsilon_t}{\sigma_\varepsilon} grad \varepsilon\right) + \frac{\varepsilon}{k}\left(C_{\varepsilon_1} P - C_{\varepsilon_2} \varepsilon\right) \tag{5}$$

k: turbulent kinetic energy; ***ε***: turbulent dissipation rate.

Where:

$$\upsilon_t = C_\mu \frac{k^2}{\varepsilon};\ \overline{u_i' u_j'} = -2\upsilon_t S_{ij} + \frac{2}{3} k\delta_{ij};\ P = 2\upsilon_t S_{ij} S_{ij};\ S_{ij} = \frac{1}{2}\left[\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i}\right]$$

Table 1: The constants for *k-ε* turbulence model

C_μ	σ_k	σ_ε	C_{ε_1}	C_{ε_2}
0.09	1	1.3	1.44	1.92

Pollutant concentration is calculated with the convective-diffusion equation:

$$\frac{\partial C_i}{\partial t} + U_j \frac{\partial C_i}{\partial x_j} = \frac{\partial}{\partial x_j}\left(K_t \frac{\partial C_i}{\partial x_j}\right) + S_i \tag{6}$$

Where C_i denotes the pollutant concentration, K_t is the eddy diffusivity coefficient; and S_i represents all sources and sinks terms.

2.1.5. Computational domain

The Figure 1 illustrates the computational domain, and building configuration. This study models reactive pollutant dispersion in a long street when the wind direction (x-direction) is parallel to the street direction. The origin of the coordinate system is located at the left bottom corner of the street in the computational domain. The domain size is 95m in the x-direction, 16m in the y-direction, 21m in z-direction.

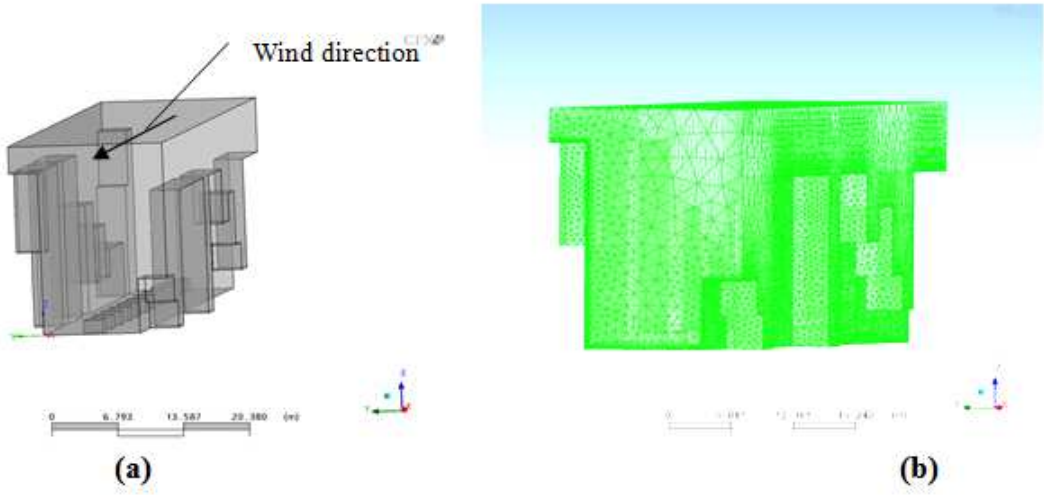

Figure 1. a) Computational domain and buildings configuration
b) Mesh of the complete computation domain.

2.2. Initialization

The emission sources considered in this study are sub-domains (volume sources), created along the street in x-direction (11 sub-domains or cars), with size of 3.5m×2m×1.48m (each car), and the distance between two cars is 5m. The vehicles were assumed to emit NO (90% of NO_x), NO_2 (10% of NO_x). We estimate the emission rate for each car, as NO emission rate of 16.5 µg/m^3s, and 2.5 µg/m^3s of NO_2. A background ozone concentration of 70µg/m^3 was then set for the entire domain [5], [3]. At the inflow boundary, wind assumed to blow along the canyon the street from east to west; with a speed of 1.5 m/s. The pressure and temperature were specified as 1 atm and 25^{0}C, respectively.

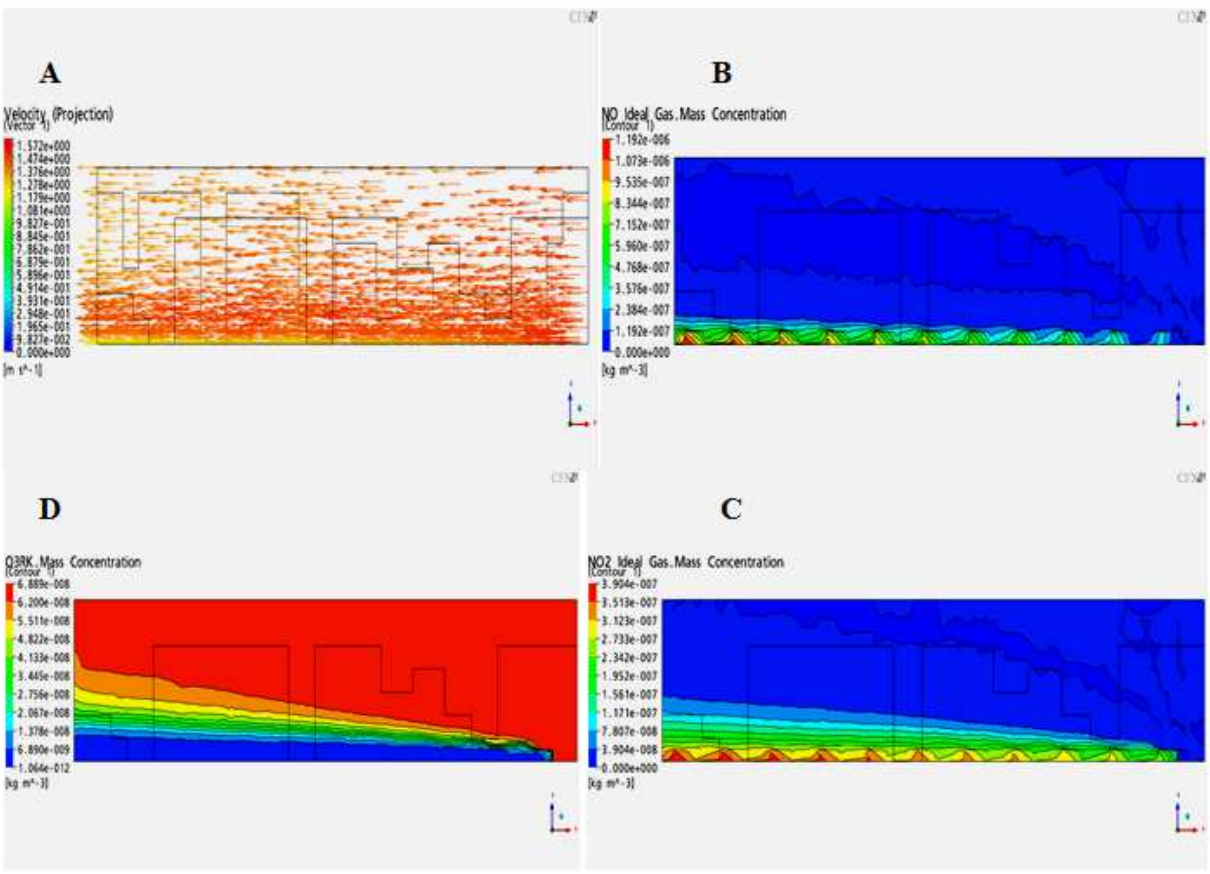

Figure 2. A) velocity vectors; B) NO, C) NO_2, and D) O_3 concentration contours on x-z plane at y=-5m (middle of street)

RESULTS AND DISCUSSION

As shown in Figure 2 the effect of wind direction was crucial and a key factor determining the dispersion of pollutants. It was very interesting to see how the concentration distribution is behaving with respect to the flow field.

Wind parallel to the street direction resulted in higher O_3 concentration levels in the middle upper area of the street (Fig.2.D). The accumulation of pollutants (NO, NO_2) along the canyon axis dominates close to the vehicular emission sources (Fig.2.B and Fig.2.C). Ozone (O_3) concentration is high apart from the upper region of the street and at inlet. This is explained by ozone rich air aloft being entrained into the canyon, followed by dispersion and reaction. A very interesting symmetric level has been occurred between ozone O_3 and NO_2 that follow opposite trends [7]. A steady rise in ozone level was observed with decreased NO_2 concentration.

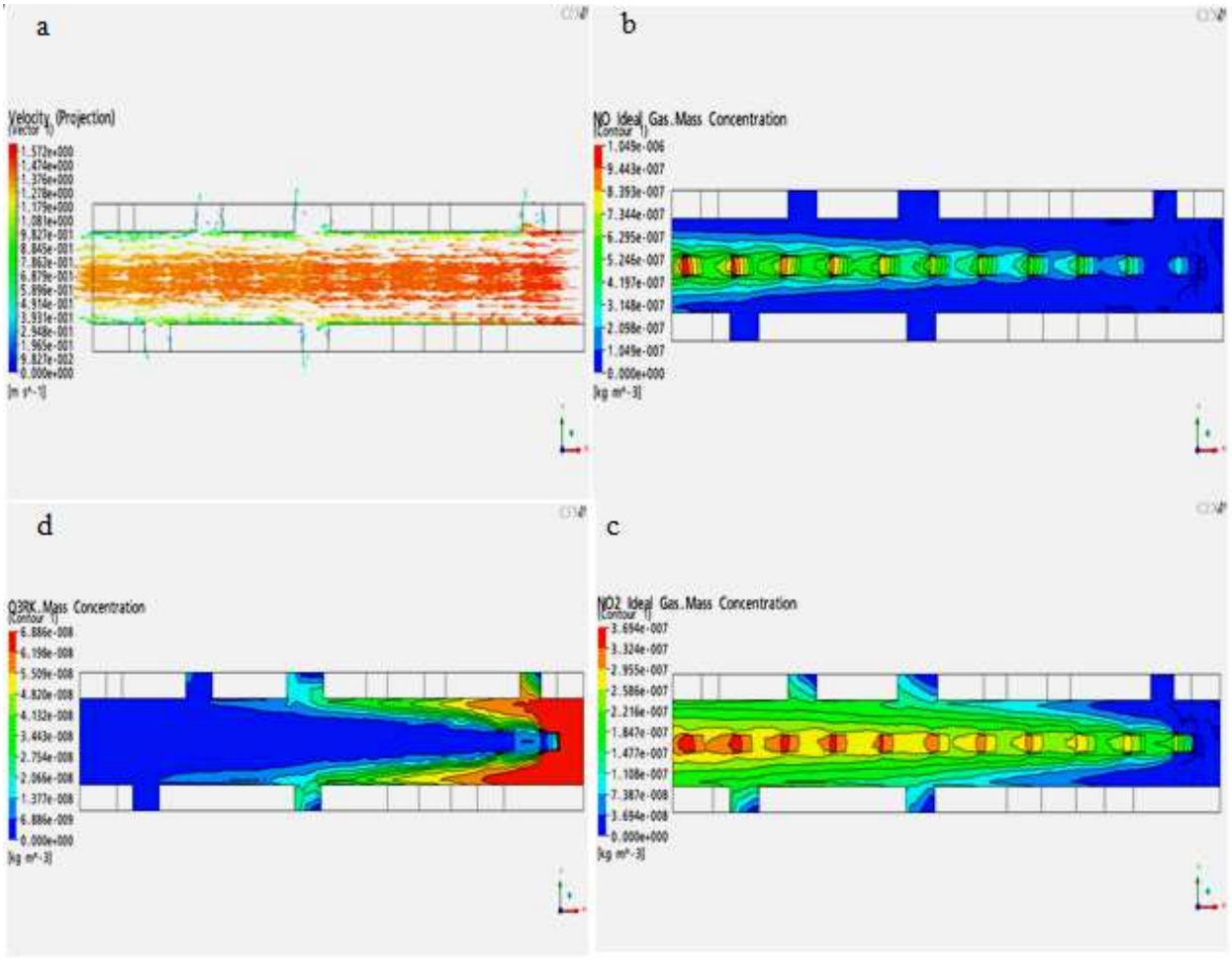

Figure 3. a) velocity vectors; b) NO concentration, c) NO_2 concentration, and d) O_3 Concentration contours on x-y plane at level z =1m (near the ground)

It is illustrated clearly that concentration of NO and NO_2 in the areas near the emission source-traffic road (Figure 3.b. and Figure 3.c), are significantly higher than that of any other areas and very low close to the buildings. The spatial distribution of NO_2 is larger than NO, because NO is quickly transformed to NO_2. Furthermore the concentration of NO and NO_2 are much lower in the inflow region than the rest of the canyon. This is in contrast with O_3 that is high at the inlet. This is explained by the consummation of ozone O_3 by NO in the street canyon to varying degrees. And the flow speed in the left side (Figure 3.a) near the ground level is weak and hence the pollutants have sufficient time spent in the mixing and reaction process of the chemical species [1]. On the other hand, there is a formation of NO_2 due to the reactions between O_3 and NO and thus, NO_2 dispersed more significantly than NO. As expected, NO and NO_2 concentration levels decrease with height while that of ozone generally increases.

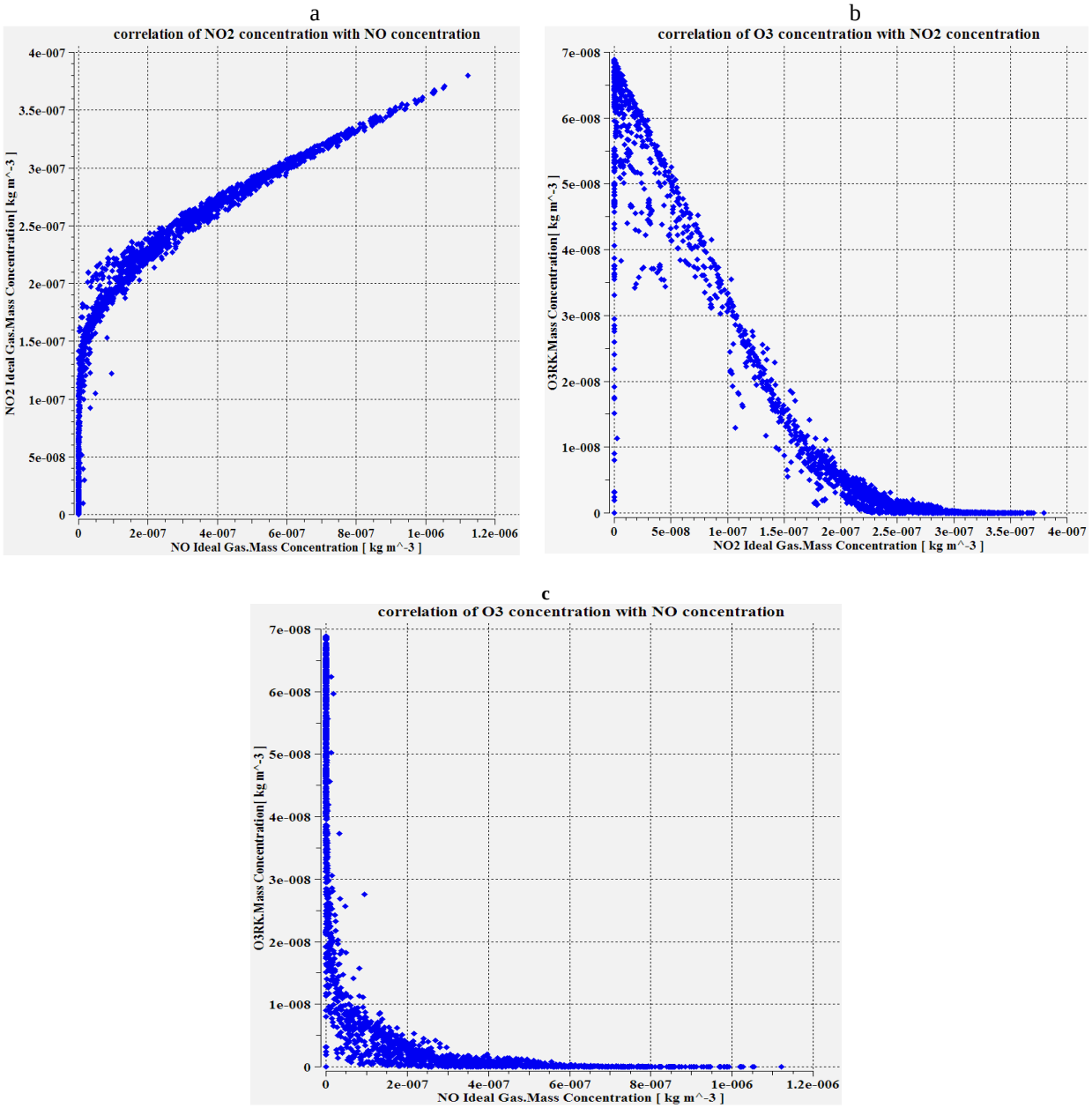

Figure 4. Domain average concentration correlation:
a)- correlation of NO_2 concentration with NO concentration.
b)- correlation of O_3 concentration with NO_2 concentration.
c)- correlation of O_3 concentration with NO concentration.

Figure 4.a shows the correlation of NO_2 concentration with NO concentration. The increasing NO_2 concentration with increasing NO concentration is displayed this variation is approximately linear above 1.5×10^{-7}kg/m^3 of NO_2 concentration, until the maximum values of NO and NO_2 concentrations, which are ~1.19×10^{-6} and ~3.9×10^{-7} kg/m^3, respectively. This case reflects the high concentration levels of NO and NO_2 near the ground, where their emission source is located. Note that the values of NO concentration is greater than NO_2 concentration, due to the rate of emission source that was assumed with a ratio one-tenth (1/10), of NO_2 to NO.

Except in the region below 1.5×10^{-7}kg/m^3 where NO_2 concentration varied between zero to 1.5×10^{-7}kg/m^3 with nearly zero NO. This was because NO_2 dispersed more than NO corresponding to areas at high levels. Because NO is quickly transformed to NO_2 (Figure 2.C and Figure 3.c).

The corresponding NO_2 and O_3 concentration levels are displayed in Figure 4.b, that shows decreasing O_3 concentration with increasing NO_2 concentration. This indicates the oxidation of NO by ozone O_3 that leads to an increase in the NO_2 concentration and linear decrease of ozone levels.

It is interesting in Figure 4.c to observe the difference between NO and O_3 concentrations. As it shown the increase of NO concentration (for $2\times10^{-7}kg/m^3$ until a maximum value) with low O_3 concentration, implies that the ozone O_3 is consumed in high degree by NO due to the reaction with it near the emission source region.

A similar behaviour is observed for O_3 concentration (more than $10^{-8}kg/m^3$) with low NO. Because O_3 concentration is high in the upper region of the street and in the inlet boundary. NO concentration was negligible in these regions. In addition there are some areas (Figure 4.c) where low O_3 concentration (less than10^{-8} kg/m^3), the NO concentration was low too (less than $2\times10^{-7}kg/m^3$). This result corresponds to areas close to building surfaces, where O_3 and NO were both considerably low, due to low wind speed and weak dispersion ability of NO. Also note that NO_2 concentration is low in these areas (Figure 2).

CONCLUSION

This study examined reactive pollutant dispersion in 3D urban street canyon in steady state. A CFD (computational fluid dynamics) code was used (ANSYS-CFX), with a standard k-ε turbulence model using transport equations for the mean concentration and concentration variance of the scalars, incorporating simple NO-NO_2-O_3 photochemistry. An area emission source of NO and NO_2 was considered in the presence of background O_3.

- The study also shows evidence that the reactive gases considered were NO and NO_2 emitted into the canyon by traffic against a background of ozone. This implied that Background ozone, transported into the canyon from inflow region (inlet), is destroyed by the NO emissions from the motor vehicles, in particular at low levels.

- The fast reaction of the emitted NO with O_3 leads to the high NO_2 concentration (because NO is quickly transformed to NO_2). In addition we observed that NO_2 dispersed more significantly than NO to higher levels, probably because it comes from both primary combustion sources within the street Canyon (direct emission from cars) and secondary formation from the NO+O_3 reaction. As a result O_3 concentration is higher at upper levels and in the region where ambient O_3 enters into the canyon, while NO and NO_2 are depleted in a high degree in these areas (Figure 2).

- The highest ozone O_3 concentration occurred under high wind speeds; the wind speed dependency becomes more distinct in Figure 2. The results indicated that there is a strong influence of the street geometry on the wind field and consequently the pollutant dispersion around the buildings surfaces.

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